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Mechanical testing and modeling in MST

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The mission of the Materials Science and Technology Division includes the development of constitutive deformation and failure models for the metals, polymers, ceramics, and composites of interest to Department of Energy, Department of Defense, and industrially-sponsored programs. To meet this mission it hosts a range of quasi-static and dynamic testing facilities. In addition to testing of common materials such as copper, steels, or polycarbonate, special facilities are used to evaluate hazardous materials, such as high explosives, beryllium, uranium, and plutonium. The experimental capabilities are augmented with models offering predictive capability and insight. Predictive constitutive models are benchmarked and validated through comprehensive experimental databases of strength and damage behavior using a suite of loading techniques and conditions including tension, compression, shear/torsion, large strain, and multi-axial stress (i.e. bending, high pressure, etc.). As the effects of processing are to critical to accurate prediction of its mechanical behavior, MST hosts a range of metallographic and characterization tools. Specific areas of expertise include understanding the effects of complex strain paths (such as shock pre-straining and load reversals), crystallographic preferred orientation (texture development), and phase transformations.

Mechanical testing activity is distributed across all four MST groups according to their respective missions. The Structure/Property Relations group (MST-8) hosts testing capability outside secure areas and modeling experts benefitting from modeling synergy with complementary basic energy science funded activity. Nuclear Materials Science (MST-16) and Polymers & Coatings (MST-7) perform actinide and polymer testing respectively. Materials Technology-Metallurgy (MST-6) is a center of excellence for manufacturing and industrial processing, with expertise specific to uranium.

Integrated testing/characterization/modeling regimen validates advanced simulations

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An integrated testing/characterization/modeling regimen, wherein mechanical properties measurements are augmented with studies of microstructure and complemented with state-of-the-art simulation providing added insight, is a hallmark of studies in MST. A good example is an ongoing collaboration with the Department of Defense in dynamic extrusion. The study addresses high-rate, large-strain, tensile-dominated deformation and exercises both constitutive strength and damage models. In this example, a copper 7.6 mm-diameter sphere is accelerated to 200 ms⁻¹ into a conical extrusion die (Figure 1a). The sample is deformed and strain localization results in necking, which is visible in high-speed photography (Figure 1b). The fragments are characterized post-mortem by techniques such as electron backscatter diffraction (EBSD), which shows microstructure and texture (Figure 1c). The experimental results are compared with continuum hydrodynamic simulations that use parameterized strength and damage models (Figure 1d). Ultimately these data are used to validate advanced simulations (Figure 1e).

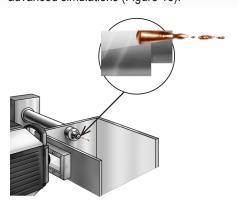


Figure 1a, conical extrusion die.

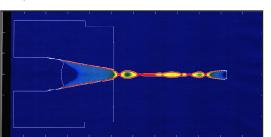


Figure 1e) Mesa 2d simulation of extrusion process.

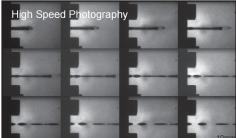


Figure 1b) High-speed photography of evolving fragmentation.

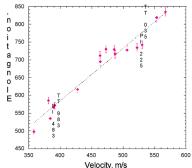


Figure 1d) Percent total elongation vs. impact velocity.

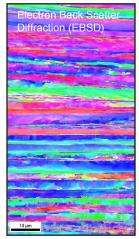


Figure 1c) EBSD measurements showing microstructure and texture.

Dynamic capability

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Equipment	Strain rate s ⁻¹	Temperature (K)	Comment
Gas guns (40, 80, 117 mm)	to 10⁵	to 1,000	VISAR instrumented; soft recovery tank; Pu rated
Split Hopkinson bars (4)	to 10 ⁴	77< <2,300	Compression and tension
Taylor anvils (2)			7-12 mm diameter, 25-40 mm length; Pu-rated
Charpy impact tester		125<, <500	Instrumented anvil; 400J capacity
Drop tower		125<, <500	5 M height

Quasistatic capability

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Equipment	Capacity (KN)	Temperature (K)	Comment		
MTS frames (12) Instron frames (9)	2-250	77-1,800	Air, vacuum, inert atmosphere; beryllium rated; hydraulic, electromechanical		
4 post crosshead mounted	10,000	Ambient	RT forging and ECAE studies		
Torsion multiaxial (MTS)	100	Ambient	120 degree 10 turn		
Bulge tester		Ambient	Formability		
Custom Instron	250	77-2,000	Horizontal geometry for neutron diffraction		
Gleeble		RT to melt	Formability and hot workability studies		

80-mm gas powder launcher

At strain-rates, approximately 10⁵ s⁻¹ and greater, microstructural and damage evolution from shock loading typically differs from that produced at lower strain rates. Specifically, plasticity occurs along a discontinu-



Figure 2a) Soft recovery tank

ous front in the shock deformation regime. To access and diagnose material response in this regime specialized equipment is needed.

One example is the 80-mm gas/powder launcher that has "soft-recovery" capability (Figure 2a), in which shocked samples are decelerated while minimizing post-shock deformation and damage. The launcher can accelerate projectiles to velocities from 200 ms⁻¹ to 1.2 kms⁻¹ (with gas), and up to 2 kms⁻¹ (with gun powder). A flyer-plate impacts on a sample embedded in an assembly that is released into a large catch tank after impact. By varying the projectile velocity, flyer and sample thicknesses, and flyer material, a range of pressures and pulse durations can be achieved. The launcher is used for studies of shock loading and spall strength. In some tests, shock pre-strained samples are recovered and subsequently mechanically tested to study shock-hardening behavior. Post-mortem characterization may involve transmission electron microscopy (TEM) investigation or serial sectioning reconstruction of the incipient spall damage network.

Standard and custom testing

A wide spectrum of ASTM standard mechanical tests are used to meet customer requirements. They include tension, compression, torsion, shear, flexure, fatigue, creep, fracture toughness, and multiaxial loading of metals, ceramics, polymers, and composites. Cryogenic and high-temperature fixtures and furnaces are available, as well as environmental chambers that control humidity. Custom fixtures and samples are routinely fabricated for specialized materials and component testing (Figure 2b). State-of-the-art diagnostics (e.g. DIC, see page 4) are applied during testing.



Figure 2b) Mechanical testing specimens, from top, tensile; multi-axial (internal pressure-tension) tubes; torsion; and losipescu shear testing.

Modeling constitutive performance

To complement experimental expertise MST Division also supports a broad capability in modeling constitutive performance.

Mechanical threshold stress model

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The mechanical threshold strength (MTS) model has proved effective in predicting the constitutive response of metals over a wide range of temperatures and strain rates. The model is based on dislocation dynamics and thermal activation theory. It describes a material's flow stress as a combination of three components: rate-independent interactions of dislocations with long-range barriers; a rate and temperature dependent contribution due to intrinsic barriers; and a structure that evolves with plastic strain due to work hardening and dynamic recovery. The parameters for the model are material specific and

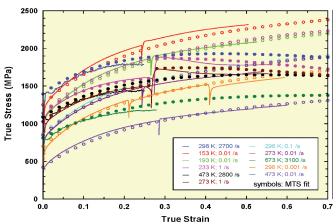


Figure 3a) Measured and fitted data.

Polycrystalline modeling

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The MTS model described above is a continuum-based model that has proven robust, especially for dynamic problems, but the next challenge for modeling is to account for heterogeneity produced by the polycrystalline nature of many materials. To do so, a suite of polycrystal codes have been developed that can account for the real deformation mechanisms of the grains (elasticity, dislocations, twins, and transformations), including texture. As a consequence, they provide a link between microscopic mechanisms and measured response. We currently use two polycrystal codes, a visco-plastic self-consistent code (VPSC) and elasto-plastic self-consistent code (EPSC).

are determined from stress-strain response measured for a range of strain rate and temperature conditions (Figure 3a). The validity of the model can be tested using Taylor impact tests, in which a right cylinder is impacted against an anvil (Figure 3b). The Taylor test is simulated using an explicit Lagrangian finite element code, incorporating the MTS constitutive modeling to describe the temperature and rate-dependent materials properties. Experimentally measured profiles are compared with simulations to establish the applicability of the model to large-scale applications (Figure 3c).

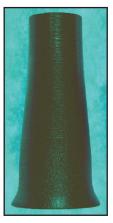


Figure 3b) Deformed lead alloy Taylor cylinder.

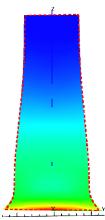
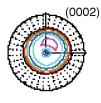
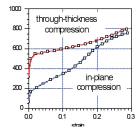


Figure 3c) Measured profile (dotted line) and predicted profile (colored plot) using MTS constitutive data.

Among the systems studied are: Zr (Figure 3d), Be, Mg, and geological systems, such as quartz and calcite. VPSC is used to simulate plastic forming and predicts yield stress, texture, and microstructure evolution associated with large strain deformation. It has been interfaced with the finite element codes for addressing complex geometries while retaining the use of a sophisticated constitutive equation. EPSC is used to simulate evolution of internal stress in metallic aggregates subjected to temperature, deformation ,and pressure. Both codes are approved for public distribution and are used in more than 100 institutions worldwide.





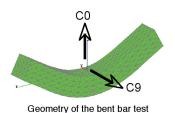


Figure 3d) Measured pole figure for rolled zirconium (left); VPSC calculation of monotonic loading of rolled zirconium (center); Four-point bend simulation of textured zirconium, using VPSC constitutive model (right).

Digital image correlation: A full-field deformation mapping technique

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MST Division hosts a range of complementary characterization tools beyond standard load cells and strain-gauges. One example is digital image correlation (DIC). This optical technique relies on the computer vision approach to extract the whole-field displacement data and is a robust, flexible approach to measuring large deformations for complicated sample geometries. It can measure in-plane displacement field on a two-dimensional planar specimen or three-dimensional displacement field on a curved surface. When used in conjunction with high-speed photography, it provides unique insights of dynamic deformation. The principle is simple. A random speckle pattern is applied to the surface of the specimen, usually by spraying black paint on a white background. By comparing variations in digital images before and after deformation (in mathematical terms this is achieved by minimizing the correlation coefficient) the stretch and rotation of the region surrounding a point can be determined. By using

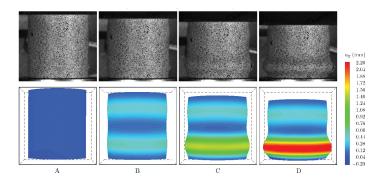


Figure 4a) DIC measurement of aluminum tube in compression. The onset and evolution of the elasto-plastic buckling are apparent.

appropriate optics and megapixel CCD cameras, strain resolutions at the level of 0.001% are achievable.

Working with hazardous materials

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MST mechanical characterization teams routinely test hazardous materials, including high explosives, actinides and beryllium. Standard capabilities include compression and tension, tensile Hopkinson bar, Taylor impact and flyer plate impact systems. With the support of local subject matter experts and industrial hygienists we develop specialized experimental techniques while maintaining personnel and environmental safety. Facilities are available in classified and unclassified environments. MST staff perform measurements on small quantities of high explosive and work closely with counterparts in DE Division (which handles larger quantities of HE, contact: Darla Thompson, dkgraff@lanl.gov). Unique measurements of preferred crystallographic orientation, phase behavior, and residual strain information are made during testing in tension, compression, or shear using the neutron beam facility at LANSCE, contact: Don Brown, dbrown@lanl.gov. MST maintains a comprehensive capability to test and characterize plutonium at TA-55 that includes the Kolsky Bar (Figure 4b). In addition, a Pu-Taylor Anvil Impact Facility is under development to validate constitutive strength models and computer codes used in weapons simulations, contact: Michael Bange, bange@lanl.gov.



Figure 4b) Kolsky Bar glovebox at TA-55's plutonium test facility.

Polymeric and soft materials

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Structure-property relationships of polymeric and other soft materials including thermoplastics, thermosets, adhesives, pottings, epoxies, urethanes, flexible and rigid foams, highly-filled polymers, copolymers, elastomers, gels, explosive binders and composites for a broad range of applications are measured in MST-7. For example, the dynamic mechanical analyzer (Figure 4c) measures elastic moduli and energy dissipative properties of materials as a function of temperature and deformation rate. It also provides information on thermal transitions and mechanical relaxation processes important for mechanical property characterization and understanding of dynamic behavior of materials.



Figure 4c) Dynamic mechanical analyzer



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